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Analyses of PEM-2 (Pollution Episodic Model Version 2) Model Evaluation Results for Short-Term Urban Particulate Matter

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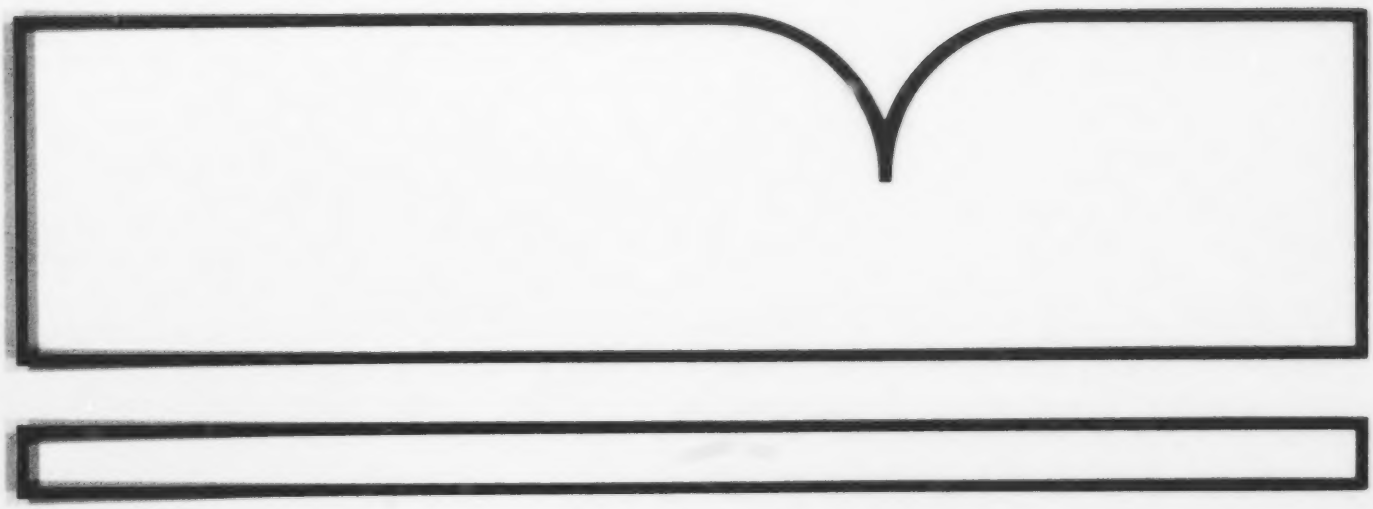

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ANALYSES OF PEM-2 MODEL EVALUATION RESULTS FOR SHORT-TERM URBAN PARTICULATE MATTER

by

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16. ABSTRACT

The Pollution Episodic Model Version 2 (PEM-2), an urban dispersion model, has been evaluated with measurements from the 1982 Philadelphia Aerosol Field Study data base in order to investigate its ability to model 12-hour average concentrations of particulate matter less than 10 micrometers (PM_{10}). Regional PM_{10} background was derived from the measured concentration at an upwind site selected as the background monitor with the modeled PM_{10} concentrations subtracted because all sites were in the emissions region. About 70% of the measured PM_{10} at most monitoring sites was contributed by regional background. Model performance was determined from statistical measures of difference and correlation between observed and modeled concentrations paired in time and location. Statistical results were better for modeled plus background values versus observed concentrations. Low correlations were found from concentration pairs composed of modeled concentrations and observed minus background values. The regional background dominated many of the evaluation statistics since it represented a large fraction of measured urban PM_{10} concentrations. Concentration estimates from PEM-2 and the RAM model are compared from independent evaluations with this data base. Mean and high-five PM_{10} concentrations from the PEM-2 model were about 25% lower than RAM predictions at four sites within the city limits, and 35-40% lower at the two most distant sites from the urban center.

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AFFILIATION

The author is on assignment to the Meteorology and Assessment Division, Atmospheric Sciences Research Laboratory, from the National Oceanic and Atmospheric Administration, U. S. Department of Commerce.

ABSTRACT

The Pollution Episodic Model Version 2 (PEM-2), an urban dispersion model, has been evaluated with measurements from the 1982 Philadelphia Aerosol Field Study data base in order to investigate its ability to model 12-hour average concentrations of particulate matter less than 10 micrometers (PM_{10}). Modeled fine (< 2.5 μm) and coarse (2.5 - 10 μm) particulate total masses were combined and then statistically evaluated against corresponding PM_{10} measurements at six monitoring sites for a 29-day experimental period.

Modeled results from urban emissions alone underestimated measured concentrations by up to a factor of 4, which revealed regional background values were large and needed to be accurately determined. Regional PM_{10} background was derived from the measured concentration at an upwind site selected as the background monitor with the modeled PM_{10} concentration subtracted because all sites were in the emissions region. About 70% of the measured PM_{10} at most monitoring sites was contributed by regional background.

Model performance was determined from statistical measures of difference and correlation between observed and modeled concentrations paired in time and location. Statistical results were better for modeled plus background values versus observed concentrations. Low correlations were found from concentration pairs composed of modeled concentrations and observed minus background values. The regional background dominated many of the evaluation statistics since it represented a large fraction of measured urban PM_{10} concentrations. Results differed based upon the method of accounting for background.

Concentration estimates from PEM-2 and the RAM model are compared from independent evaluations with this data base. Mean and high-five PM_{10} concentrations from the PEM-2 model were about 25% lower than RAM predictions at four sites within the city limits, however, PEM-2's results were 35-40% lower at two most distant sites from the urban center. These differences in model results are attributed to particulate removal by dry deposition and settling processes in PEM-2 and the different treatments of area source emissions by these models. Results of statistical measures were still quite similiar for both models. Due to the dominant role of regional background concentrations in this evaluation study, it was not possible to conclude which model performed more accurately or that the PEM-2 provided any clear advantage over the RAM model results.

CONTENTS

Abstract iii
Figures vi
Tables vii
Acknowledgement viii

1. INTRODUCTION 1
    Model Overview 2

2. MODEL EVALUATION DATA BASE 3
    Emissions 3
    Particulate Measurements 5
    Meteorological Parameters 8

3. MODEL EVALUATION RESULTS AND DISCUSSION 12
    Model Calculation Procedures 12
    Regional Background Component 13
    Model Evaluation Statistical Results 19
    Comparative Results for the PEM-2 and RAM Models 25

4. SUMMARY AND CONCLUSIONS 32

5. REFERENCES 34

APPENDICES
    A Evaluation of Modeled Mixing Heights with PAFS Observations ... 36
    B Definitions of Statistical Measures 39
    C Observed and PEM-2 Modeled PM_{10} Concentrations 41

FIGURES

Number		Page
1	Area emissions grid and PEM-2 model calculation grid for the Philadelphia evaluation. Dashed line denotes the city limit and the numbered locations are the six PAFS sites.	4
2	Map of the Philadelphia metropolitan area and the locations of the PAFS particulate monitoring sites and Philadelphia International Airport (PHL) where meteorological observations were taken.	6
3	Temperature (solid) and humidity (dashed) profiles for A) before sunrise and B) mid-afternoon on on 3 August 1982 at the Camden (CAM) site.	9
4	Time series of PM_{10} measurements (dashed) and modeled (solid) concentrations (without background) averaged over all sites for each 12-hour period of the PAFS study period. Day 1 to 30 corresponds to 16 July through 15 August 1982.	16
5	Observed versus model predicted (plus background) PM_{10} concentrations at all sites over all periods. The proposed 24-hour standard for PM_{10} is 150 $\mu g/m^3$.	21

TABLES

Number		Page
1	Averaged day and night total emission rates from area and point sources from the Philadelphia emissions inventory	5
2	Philadelphia Aerosol Field Study monitoring site information	7
3	Observed mixing heights from the 1982 PAFS period	11
4	Deposition and settling velocities for the PEM-2 evaluation runs	12
5	PM_{10} concentrations at the PAFS monitoring sites	14
6	Results of 12-hour averaged wind speed and direction and PM_{10} measured at the upwind site during PAFS.	17
7	Observed and model predicted PM_{10} at upwind sites	18
8	PEM-2 evaluation statistics for PM_{10} (Set 1)	20
9	Statistical results for each PAFS site for PM_{10} (Set 1)	23
10	PEM-2 evaluation statistics for PM_{10} (Set 2)	24
11	Statistical results for each PAFS site for PM_{10} (Set 2)	26
12	PEM-2 and RAM model results for PM_{10}	28
13	Comparison of PEM-2 and RAM for PM_{10} at the PAFS sites	30
14	Comparison of high-five PM_{10} concentrations for PEM-2 and RAM	31
A-1	Statistical results of mixing height model evaluation	38

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SECTION 1

INTRODUCTION

The proposed National Ambient Air Quality Standards (NAAQS) regulations will establish a 24-hour standard for particulate matter in the size range less than 10 micrometers (PM_{10}). Once this short-term standard is promulgated, state and local regulatory agencies will be required to develop implementation plans to attain and maintain the new standards. Air quality dispersion models are expected to be relied upon for urban regulatory applications and emission control strategies contained in the state implementation plans. EPA has issued the Guideline on Air Quality Models (Revised) which contains recommended procedures and models for various applications (EPA, 1986). The evaluation of a dispersion model with existing measurements is advocated to determine its applicability and accuracy in modeling particulates in urban environments.

In support of the Agency's policy to regulate urban particulates, the Atmospheric Sciences Research Laboratory has sponsored the development and evaluation effort of the Pollution Episodic Model Version 2 (PEM-2). The PEM-2 is an urban-scale Gaussian plume diffusion-deposition model which has been designed to compute short-term (up to 24-hours) ground-level concentrations of one or two species of particulate or gaseous pollutants. The model accounts for the transport, dispersion, and the deposition and settling processes of particulates from multiple point and/or area emission sources. The technical features and complete instructions of the PEM-2 model are contained in Rao (1986).

Two evaluation efforts have been conducted on different versions of this model. Pendergrass and Rao (1984) present the statistical results when the original version (PEM) was applied to a selected particulate data set from the St. Louis Regional Air Pollution Study. The current version of the model, designated as PEM-2,has been recently evaluated against measurements from the Philadelphia Aerosol Field Study (Ku and Rao, 1986). In this evaluation, separate model calculations were made for fine particle (< 2.5 μm) and coarse particle (2.5 - 10 μm) total masses and statistical measures for observed and calculated concentrations were determined for each size range. However, there is a need to know

the ability of PEM-2 to estimate PM_{10} concentrations and how its performance compares to that of other dispersion models.

This report contains the results of various analyses to evaluate the ability of PEM-2 to model PM_{10} concentrations. The model results for fine and coarse particulates from Ku and Rao (1986) were aggregated and statistically evaluated against corresponding PM_{10} measurements derived from observed fine and coarse particulate concentrations from the Philadelphia data base. Statistical measures of difference and correlation for modeled and measured concentrations paired in time and space were used to examine model performance. In addition, comparative results from PEM-2 and RAM, a model recommended in the EPA guideline for urban applications, are presented. Results of analyzing the regional background component are also described in order to assess its contribution and role in urban particulate model evaluation.

MODEL OVERVIEW

The PEM-2 model is designed for short-term urban scale applications since it is limited to 24 one-hour scenarios and a 50-km domain. It is capable of calculating ground-level concentrations and deposition fluxes of one or two particulate or gaseous species over a uniform model receptor grid from a maximum of 300 point sources and/or 50 area sources.

Since Rao (1986) provides a comprehensive description of the model, only the notable features that distinguish PEM-2 from other urban Gaussian plume models are discussed. The important advancements incorporated into the PEM-2 model are the realistic, yet practical methods of simulating dry removal processes and chemical transformation. Dry deposition and gravitational settling of particulates are modeled through analytical solutions of the gradient transfer equations (Rao, 1984). Deposition and settling velocities are specified by the user. If these processes are not considered, the model equations reduce to the familiar Gaussian plume diffusion algorithms. The PEM-2 also contains an option to consider the new plume rise/ penetration methods of Briggs (1984) for unstable-neutral conditions, however, the standard Briggs plume rise equations and the all or no penetration scheme are the default methods. In PEM-2, the contributions from a particular area source are numerically determined to impact the concentrations at 9 downwind receptor grid cells, which in many cases may not extend to the model boundary. Otherwise, PEM-2 is consistent with other Agency models in its treatment of various technical features and processes.

SECTION 2

MODEL EVALUATION DATA BASE

All the measurements necessary to perform a model evaluation for urban particulates were obtained during the Philadelphia Aerosol Field Study (PAFS). The PAFS field program was conducted during an intensive 31-day period from 14 July to 14 August 1982 in the metropolitan region of Philadelphia, Pennsylvania. Brief descriptions of the emission inventory, particulate measurements, and meteorological parameter observations used in the model evaluation are provided since complete details have been documented in the reports cited herein.

EMISSIONS

A comprehensive inventory of fine (FP) and coarse (CP) particulate total mass emissions was developed specifically for the experimental period. Some real-time sampling was performed and an effort was made to determine whether important sources were operating continuously or off-line at times during the study period. Nevertheless, it is ackowledged that the hourly emissions were primarily derived from long-term values and should not be construed to represent actual emissions measurements (Toothman et al., 1985).

The components of the inventory included 300 major point sources, 289 area sources, gridded mobile sources, gridded minor point sources, and 25 sources of Industrial Process Fugitive Particulate Emissions (IPFPE). The area, gridded mobile, and minor point source emissions were combined into a single file for input to the model because they were constructed on the same 17 X 17 grid with individual cell sizes of 2.5 km on a side. The IPFPE sources were also incorporated into this emissions grid where each existed, although their grid cell sizes were either 0.2 km or 0.5 km. The 42.5 km by 42.5 km area emissions grid is shown inside the larger PEM-2 model calculation domain in Figure 1.

The model grid was enlarged to 80 km by 80 km to accommodate the 50 out of the 300 major point sources located outside the area source grid. A list of the major point sources reveals that the top 50 sources contributed about 50% of the point source particulate emissions (Toothman et al., 1985). The tallest stack in Philadelphia was 152 m, however, most stack heights were under 100 m.

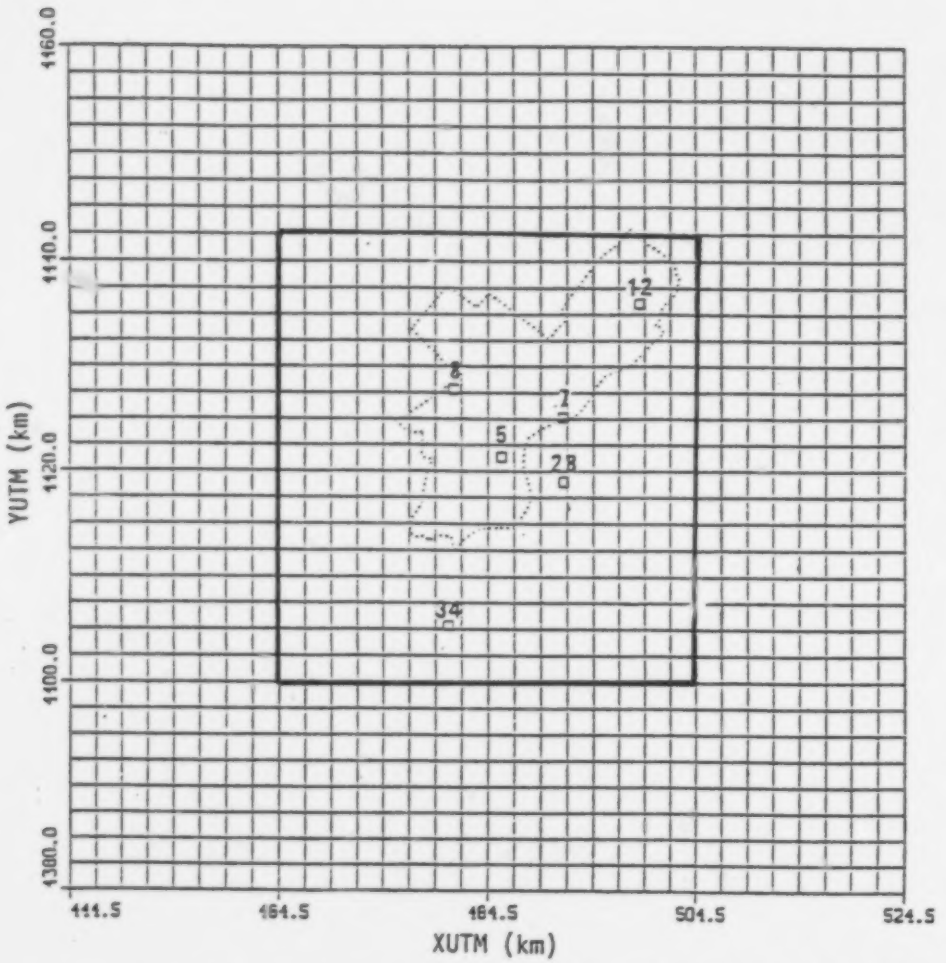

Figure 1. Area emissions grid and PEM-2 model calculation grid for the Philadelphia evaluation. Dashed line denotes the city limit and the numbered locations are the six PAFS sites.

Additionally, the point sources were generally distributed along the Delaware River which is oriented in a nearly NE-SW line through the middle of the model domain (Figure 2). Table 1 reveals that point sources represent an important part of the total particulate emissions in both size ranges in Philadelphia.

TABLE 1. AVERAGED DAY AND NIGHT TOTAL EMISSION RATES FROM AREA AND POINT SOURCES IN THE PHILADELPHIA METROPOLITAN AREA

POLLUTANT	AREA EMISSIONS (kg/s)		POINT EMISSIONS (kg/s)	
	DAY	NIGHT	DAY	NIGHT
FP total mass	7.897	3.021	4.269	3.724
CP total mass	5.133	1.668	1.737	1.536

DAY = 12-hour period starting at 0600 EDT
NIGHT = 12-hour period starting at 1800 EDT
Reference - Ku and Rao (1986)

Diurnal curves in Ku and Rao (1986) indicate that area source particulate emissions were indeed greater than those from point sources during the daytime period. FP and CP area emissions displayed a significant increase and decrease during the early morning and late afternoon periods, respectively, which are associated with large changes in traffic volume and some industrial activity.

PARTICULATE MEASUREMENTS

There were six PAFS monitoring sites equipped with dichotomous filter samplers which provided continuous FP and CP measurements during the 31-day experimental study. Information about the instrumentation, data reduction, and quality control and assurance procedures are contained in PEDCO (1983). The location of each site is shown in Figure 2 and detailed information is also provided in Table 2. All 6 sites were located within the urban emissions region and 4 sites (i.e. BRD, FRB, WTP, ARP) were situated inside the city limits. Site BRD is centrally located in the downtown area. Sites ARP and CLK are the most distant monitors from the city at 19.7 km and 16.7 km, respectively, with site BRD's location as the reference position. Site CLK is situated in the most remote

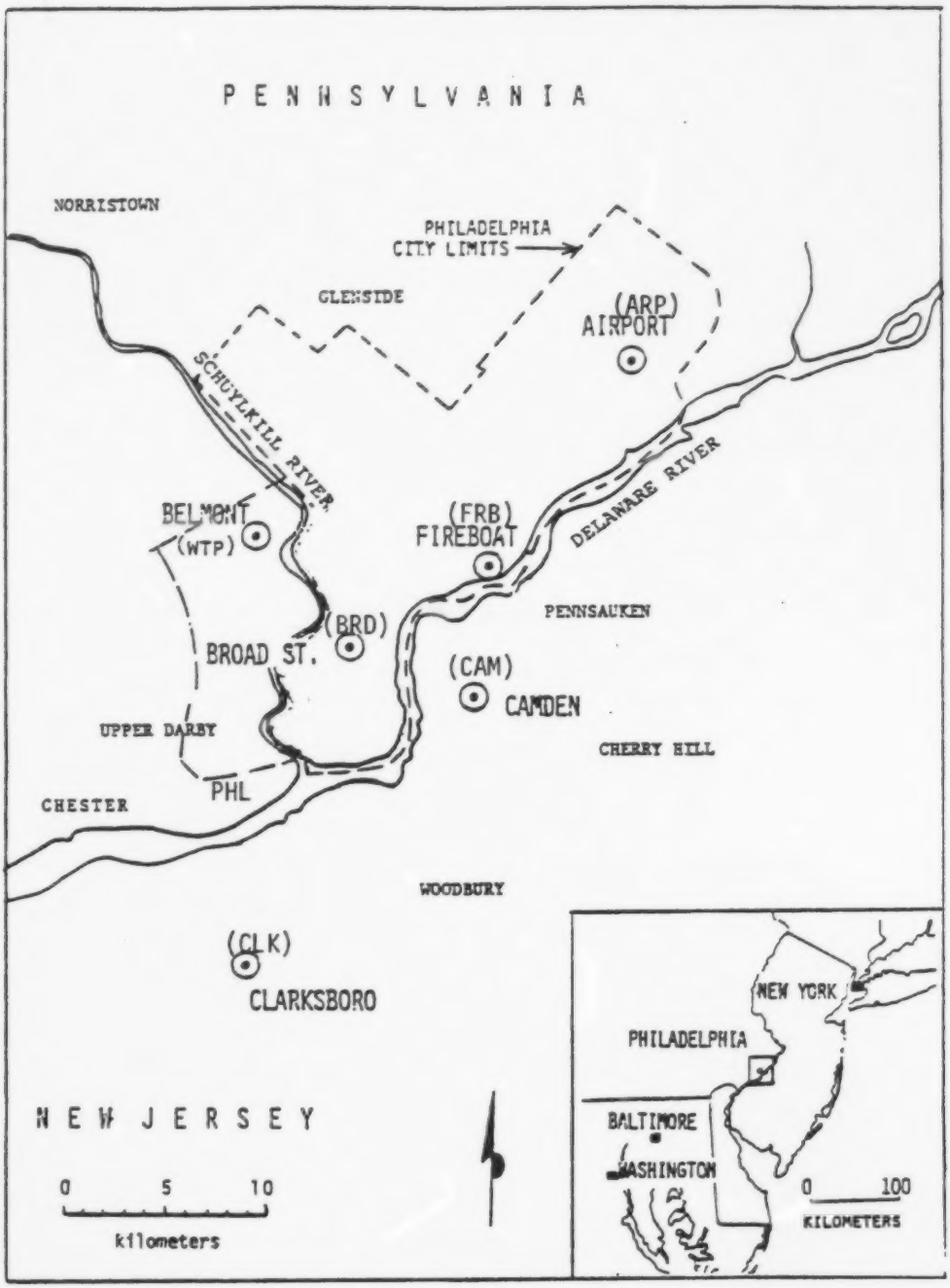

Figure 2. Map of the Philadelphia metropolitan area and the locations of the PAFS particulate monitoring sites, and Philadelphia International Airport (PHL) where meteorological observations were taken.

TABLE 2. PHILADELPHIA AEROSOL FIELD STUDY MONITORING SITE INFORMATION

SITE	ABBREVIATION	LOCATION	UTM* COORDINATES (km)	DISTANCE† (km)
5	BRD	Community Health Service Bldg. 500 South Broad Street (Urban/commercial)	4421.35 N 485.81 E	----
7	FRB	Fireboat Station Allegheny Ave. & Delaware River (Suburban/industrial)	4425.17 N 491.67 E	7.0
8	WTP	Water Treatment Plant Ford Road & Belmont Ave. (Suburban/residential)	4427.83 N 481.20 E	8.0
12	ARP	Northeast Airport Grant & Ashton Roads (Suburban-rural)	4436.02 N 498.97 E	19.7
28	CAM	Inst. for Medical Research Copewood & Davis Streets Camden, NJ (Suburban/residential)	4419.00 N 491.70 E	6.3
34	CLK	Shady Lane Home Cohawkin and County House Roads Clarksboro, NJ (Suburban-rural)	4405.40 N 480.70 E	16.7

† Distance is from Site BRD

* UTM - Universal Transverse Mercator northing (N) and easting (E) in Zone 18

setting south of the city with nearby rural surroundings (Figure 2).

The FP and CP total mass measurements consisted of 12-hour average concentrations. The two averaging periods of 0600-1800 EDT and 1800-0600 EDT are essentially representative of daytime and nighttime conditions, respectively.

METEOROLOGICAL PARAMETERS

The model requires hourly values of wind speed and direction, temperature, mixing height, and stability class. Since there were long periods of missing data from the meteorological instruments at each site, none of these data was used in this evaluation. Consequently, hourly surface observations made by the National Weather Service at the Philadelphia International Airport (PHL) located in the southwest section of the city were obtained for the model evaluation. It is recognized that these data do not represent hourly averaged conditions, and a single point measurement greatly simplifies the complex spatial and time varying flow patterns expected over an urban region. Nevertheless, in many model applications, such observations are relied upon when quality-assured on-site meteorological data are lacking.

High resolution upper air temperature and relative humidity measurements up to 2000 m were obtained by an airsonde system (PEDCO, 1983) which was launched three times daily at 0400, 1000, and 1600 EDT from 16 July through 14 August at the CAM site. The height of the lowest elevated temperature inversion base defined the mixing height, Z_i. Example morning and afternoon profiles are shown in Figure 3 to illustrate the large variation in Z_i over the daytime period. In a few cases when no inversion existed (in some afternoon profiles), Z_i was determined as the base height of a stable, dry layer which was found where the product of the temperature and humidity gradients was a maximum negative value.

The near-sunrise temperature profile in Figure 3 reveals that an elevated nocturnal inversion capped the shallow urban boundary layer (UBL), a common feature of the temperature structure over cities (Godowitch et al., 1985). However, there was large variability in the low level morning temperature structure at this site over the experimental period because of its position outside of the central urban area. When this site was downwind, the UBL was often situated between a shallow surface-based inversion and an elevated nocturnal inversion.

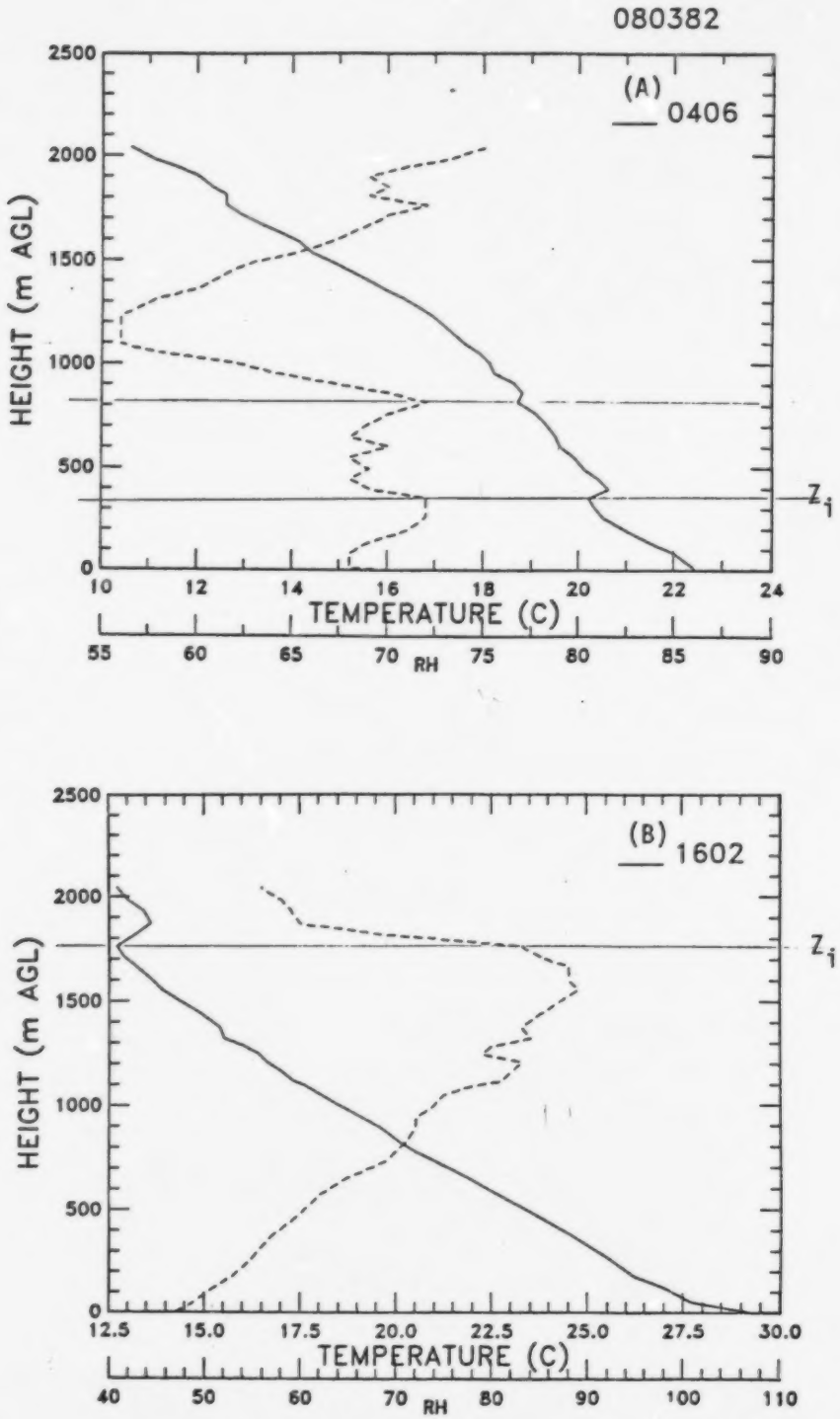

Figure 3. Temperature (solid) and humidity (dashed) profiles for A) before sunrise and B) mid-afternoon on 3 August 1982 at the Camden site.

Thus, early morning profiles at the CAM site exhibited the same features in the vertical extent and structure of the UBL as suburban locations described by Godowitch et al. (1987). Since the CAM site was the only upper air site, some morning urban Z_i's were defined as the height of the elevated UBL top when a surface inversion existed at this site. It is recognized that Z_i is spatially variable in the urban area at this time, but a zero Z_i is unrealistic since surface-based nocturnal inversions are rare in the central city.

Table 3 lists the Z_i observations for each time over the study period. There were large differences in Z_i as values ranged from 100 m to 898 m at 0400 EDT and 656 m to 2100 m at 1600 EDT. The observed morning and afternoon mixing heights, and hourly surface observations were input to the RAMMET meteorological processor (Turner and Novak, 1978) in order to derive hourly values of Z_i and stability class required by PEM-2.

The observed Z_i's at 1000 EDT provided an interesting data set for comparison with derived values from RAMMET and with those computed from an empirical urban mixing height equation (Godowitch et al., 1985). The statistical results are presented in Appendix A. A notable result was that RAMMET mixing heights were generally higher and displayed an overall positive bias when compared to observed values or those from the empirical equation. However, strong conclusions from such an evaluation of modeled and non-averaged point measurements must be tempered because the time period around 1000 is transient and often characterized by rapid growth and large variations in Z_i over very short periods as the nocturnal inversion is eroded. Additionally, this data set is a relatively small sample and limited in extent. Nevertheless, the results provide some evidence about the performance of these mixing height models for this important time period.

TABLE 3. OBSERVED MIXING HEIGHTS FROM THE 1982 PAFS PERIOD

		TIME (EDT)		
DATE	STUDY DAY	0400	1000	1600
7/16	1	301	551	1265
7/17	2	119	556	1444
7/18	3	203	365	2000 E
7/19	4	296	749	1987
7/20	5	172	354	1556
7/21	6	465	1001	1710
7/22	7	167	804	1719
7/23	8	134	186	988
7/24	9	100 E	780	2022
7/25	10	114	521	1968
7/26	11	353	1340	1967
7/27	12	100	500	1873
7/28	13	100 E	893	1851
7/29	14	898	930	1570
7/30	15	100	164	1273
7/31	16	477	1195	1709
8/01	17	305	361	1929
8/02	18	112	441	1977
8/03	19	356	685	1762
8/04	20	172	991	1831
8/05	21	199	649	1944
8/06	22	407	723	811
8/07	23	487	550	1885
8/08	24	372	372	1374
8/09	25	896	517	1290
8/10	26	544	850	1929
8/11	27	539	561	656
8/12	28	318	638	2100
8/13	29	333	374	1850
MEAN & STD DEV.		331 m ± 215	641 m ± 283.	1651 m ± 382.

E - estimated value due to missing data; not used to compute means.

SECTION 3

MODEL EVALUATION RESULTS AND DISCUSSION

MODEL CALCULATION PROCEDURES

Minor modifications of the program code were needed prior to the model runs. The area source array size of 50 was increased to 289 in order to include the entire area emissions inventory. In addition, code changes were made in the calculations of the concentrations from point sources. Computations were performed only at the four grid receptors surrounding each PAFS site. Model run time was significantly reduced since calculations were made at only 24 of 1024 receptor points in the 32 X 32 model grid.

The technical features and options chosen for the model runs included; urban wind profile exponents, stack-tip downwash, new plume rise/penetration methods, and a constant height of 10 m was specified for all area sources (Ku and Rao, 1986). The deposition (V_d) and gravitational settling (W) velocities for the particulate species are given in Table 4. These values are believed to be representative

TABLE 4. DRY DEPOSITION AND SETTLING VELOCITIES FOR THE PEM-2 EVALUATION RUNS

Particulate Range	V_d (cm/s)		W (cm/s)	
	Day	Night	Day	Night
Fine (FP)	0.2	0.1	0.0	0.0
Coarse (CP)	0.5	0.5	0.25	0.25

for each size range, however, there is uncertainty since there is a lack of experimental deposition measurements in urban areas. Nevertheless, these estimates provide for differences between the time periods and for different size ranges.

PEM-2 was executed to compute hourly concentrations of FP and CP due to hourly emissions and hourly meteorological parameters for the 29-day period from 16 July through 14 August 1982. Modeled concentrations were stored on

magnetic tape for post-processing into 12-hour averages. The modeled concentration at each PAFS site was determined as the weighted average of the four surrounding gridded receptor values because PEM-2 does not allow for input of non-gridded receptor coordinates. Although background values may be input to the model, background concentrations were not considered in the evaluation runs. Consequently, the modeled concentrations represent the urban source contribution only. The regional background was accounted for in the evaluation analyses.

REGIONAL PARTICULATE BACKGROUND COMPONENT

The determination of the regional particulate component is expected to be an important factor of urban PM_{10} modeling because it may be a relatively large fraction of the total measured concentration at urban receptor sites. This is particularly pertinent for Philadelphia because it is one in a string of large urban areas along the northeast corridor where regional pollutant transport is an important modeling consideration. The regional background measurement must be representative of the incoming concentration into an urban domain. Hence, it should be measured at an upwind site or suitable 'remote' location that is not impacted by nearby sources or influenced by emissions from the urban area being modeled. Unfortunately the PAFS sites, as noted earlier, were all located inside the Philadelphia emissions area. Thus, each site was impacted to a different extent based on its relative position within the emissions domain. However, no other PM_{10} monitoring sites were available to provide a measure of the regional background. In the evaluation performed by Ku and Rao (1986), the lowest FP and CP concentrations at one of the 4 outer sites (BRD and WTP were omitted) were selected for each 12-hour period as representative of the background values for each species.

Before describing the method to derive regional background, the actual differences in the PM_{10} concentration among the PAFS sites were found from periods when measurements were available at all sites. The number of samples varied from only 36 at the BRD site to 56 at the CAM site. Of the 58 cases between 16 July and 14 August, the results in Table 5 were determined from 29 periods when all sites were operational. With the exception of site FRB which exhibited the highest mean values since it was known to be strongly impacted by nearby fugitive sources, differences in the means were about 25% or less for the other five sites.

TABLE 5. PM_{10} CONCENTRATIONS ($\mu g/m^3$) AT THE PAFS MONITORING SITES

	SITES					
TOTAL	BRD	FRB	WTP	ARP	CAM	CLK
N	29	29	29	29	29	29
MEAN	46.1	65.8	45.9	43.8	41.0	36.5
±SD	16.9	25.1	16.7	16.2	16.9	14.3
DAY						
N	15	15	15	15	15	15
MEAN	48.1	73.3	45.5	43.8	43.1	37.6
±SD	20.5	28.4	18.7	19.8	20.1	14.4
NIGHT						
N	14	14	14	14	14	14
MEAN	44.0	57.8	46.2	43.9	38.9	35.3
±SD	12.4	18.7	15.0	12.0	13.2	14.6

N = number of concurrent measurements at all six sites
SD = standard deviation

The lowest PM_{10} concentrations occurred at the CLK site, the station furthest south of the city. The difference in PM_{10} concentrations between CLK and an urban site with the 2nd highest values was only about 10 $\mu g/m^3$. Mean values for the 12-hour nocturnal period were slightly lower than daytime values at some sites.

The relative similarity in magnitude and correspondence in the day-to-day variation in PM_{10} among these sites suggested that concentrations were strongly influenced by meteorological conditions and the regional background concentration; two factors impacting the entire urban domain. The time series of observed and model predicted concentrations averaged over all sites for each period are displayed in Figure 4. Clearly, observed PM_{10} concentrations exhibited much greater variability and their magnitudes were 2 to 4 times larger than model results. Furthermore, the modeled PM_{10} series appears to be uncorrelated with the observations. Recall that model results were computed with emissions, meteorological parameters and other physical processes; however, the incoming concentration at the upwind model boundary (i.e. background) was not included in the model runs. Therefore, regional particulate background must be accurately accounted for in the model evaluation analysis process since these results indicate that it is a large contribution to the observed PM_{10} concentrations.

The hourly surface wind observations were averaged over 12-hour intervals corresponding to the time period of the measured concentrations in order to determine which site was upwind of the city. Table 6 contains the 12-hour averaged wind speed and direction and their standard deviations over each time interval. It is evident that there were several cases exhibiting significant wind direction shifts. Nevertheless, the upwind site was selected based on the mean wind direction for the period. Sites ARP, CAM, CLK, and WTP were considered upwind under northerly, easterly, southerly, and westerly wind flows, respectively. The upwind site and its PM_{10} measurement are also given in Table 6. Both BRD and FRB sites were omitted as potential upwind sites due to their central locations within the city.

The results for each upwind site in Table 7 reveal that southerly and westerly flows were the most numerous during the study period as the WTP or CLK sites were most frequently upwind. Furthermore, upwind PM_{10} concentrations were higher and more variable under these wind flows. The lowest concentrations occurred under easterly flows. The modeled PM_{10} concentrations for each site are also shown in Table 7. As noted earlier, modeled values were expected to be different at each upwind site. The CAM site exhibited the highest modeled concentration of all upwind sites. It was furthest from the upwind model

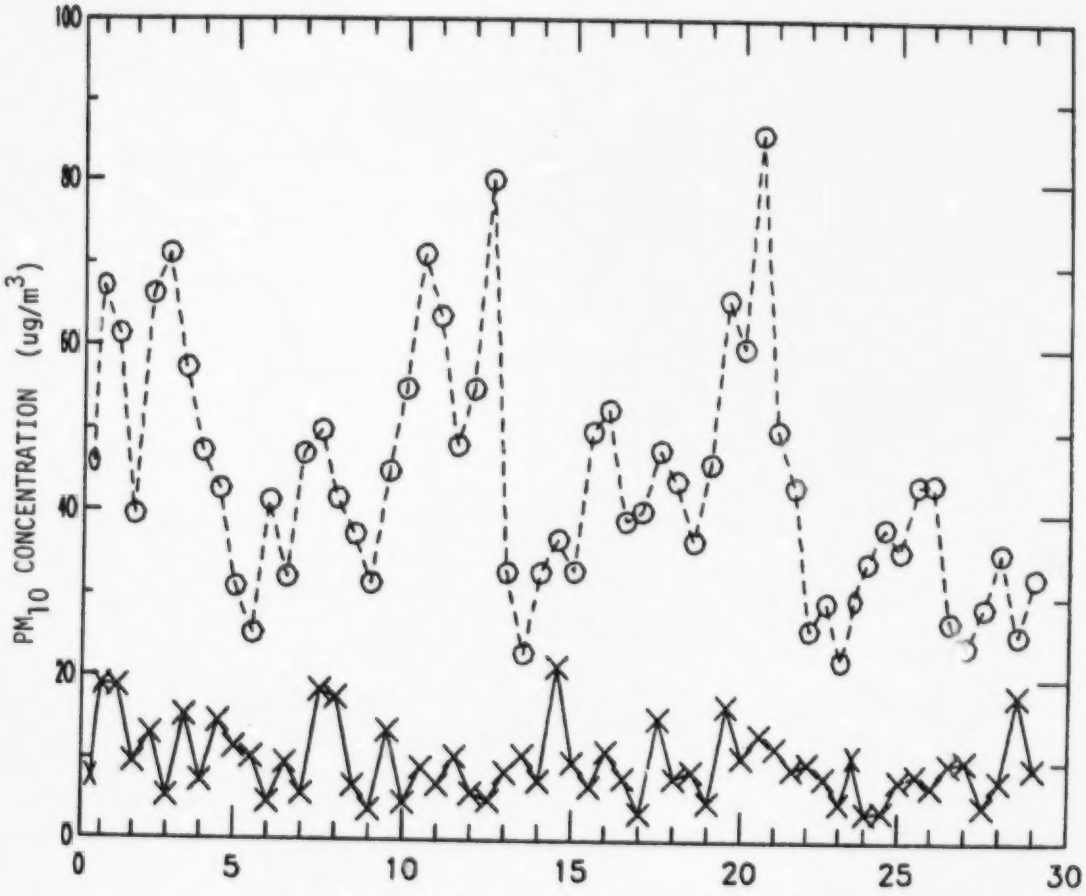

Figure 4. Time series of PM_{10} measurements (dashed) and modeled (solid) concentrations (without background) averaged over all sites for each 12-hour period of the PAFS study period. Day 1 to 30 corresponds to 16 July to 15 August 1982.

TABLE 6. RESULTS FOR 12-HOUR AVERAGED WIND SPEED AND DIRECTION AND PM_{10} CONCENTRATIONS AT THE UPWIND SITE DURING PAFS

DATE Mon/Day	START TIME (EDT)	WS (m/s)	WD (DEG)	SITE	PM_{10} (ug/m^3)	PRECIP. CASES
7/16	06	1.8±0.6	225.±24.	CLK	34.1	
7/16	18	2.4±0.8	218.±19.	CLK	M	
7/17	06	3.4±1.3	234.±14.	CLK	35.2	
7/17	18	3.0±0.7	218.±16.	CLK	28.3	
7/18	06	3.9±0.8	252.±20.	WTP	57.1	
7/18	18	3.0±0.7	233.±10.	CLK	61.5	
7/19	06	3.5±0.6	268.±29.	WTP	55.6	
7/19	18	2.7±0.8	262.±18.	WTP	43.3	X
7/20	06	4.0±1.2	320.±74.	WTP	40.3	X
7/20	18	3.2±0.6	3.±23.	ARP	33.2	
7/21	06	4.2±0.7	9.±24.	ARP	29.0	
7/21	18	3.2±0.5	319.±20.	WTP	25.8	
7/22	06	4.1±0.9	316.±18.	WTP	28.2	
7/22	18	2.0±0.8	252.±103.	WTP	28.2	
7/23	06	2.7±0.7	157.±86.	CLK	39.0	X
7/23	18	3.2±0.7	318.±63.	WTP	37.2	
7/24	06	4.5±1.4	98.±63.	CAM	M	
7/24	18	2.9±0.9	243.±48.	CLK	20.7	
7/25	06	4.2±1.5	246.±19.	CLK	34.1	
7/25	18	4.0±0.6	226.±14.	CLK	45.2	
7/26	06	3.7±1.1	282.±23.	WTP	70.5	
7/26	18	3.0±0.8	328.±44.	WTP	68.0	
7/27	06	3.0±1.0	134.±92.	CAM	50.9	
7/27	18	3.0±1.1	169.±59.	CLK	53.1	X
7/28	06	4.6±1.8	184.±49.	CLK	76.7	X
7/28	18	3.8±1.0	313.±10.	WTP	31.1	
7/29	06	4.2±0.7	313.±20.	WTP	25.5	
7/29	18	1.8±0.7	284.±45.	WTP	41.2	
7/30	06	3.8±1.1	186.±24.	CLK	25.8	
7/30	18	1.8±0.9	170.±20.	CAM	32.1	X
7/31	06	3.1±1.4	255.±76.	CLK	47.1	
7/31	18	3.2±0.9	250.±56.	CLK	39.9	
8/01	06	3.9±0.6	328.±13.	WTP	41.5	
8/01	18	2.4±0.8	289.±23.	WTP	38.3	
8/02	06	2.7±0.9	284.±42.	WTP	46.6	
8/02	18	3.0±0.7	331.±36.	WTP	47.2	
8/03	06	4.2±0.5	3.±17.	ARP	29.8	
8/03	18	2.5±1.0	340.±17.	ARP	40.1	
8/04	06	2.9±1.0	258.±55.	ARP	46.1	
8/04	18	3.1±0.8	209.±16.	CLK	49.6	
8/05	06	4.0±0.7	239.±15.	CLK	66.5	X
8/05	18	3.1±1.5	326.±79.	WTP	51.5	X
8/06	06	5.3±0.5	93.±37.	CAM	36.6	
8/06	18	3.5±0.8	86.±35.	CAM	23.7	
8/07	06	3.5±1.1	172.±75.	CAM	24.3	
8/07	18	3.3±0.7	225.±18.	CLK	16.4	X
8/08	06	4.1±0.8	188.±9.	CLK	26.5	
8/08	18	3.6±1.0	192.±48.	CAM	34.2	X
8/09	06	4.7±0.8	238.±14.	CLK	27.5	X
8/09	18	3.3±1.0	225.±20.	CLK	27.5	X
8/10	06	4.2±1.4	257.±23.	WTP	44.0	
8/10	18	3.1±1.2	334.±34.	WTP	46.4	
8/11	06	4.8±0.9	31.±19.	WTP	25.3	X
8/11	18	3.7±0.8	32.±23.	CAM	18.9	X
8/12	06	4.4±.10	38.±37.	ARP	29.6	
8/12	18	2.2±0.6	1.±14.	ARP	35.6	
8/13	06	3.0±0.7	332.±33.	ARP	26.9	
8/13	18	2.6±0.6	288.±21.	WTP	31.2	
					38.7±13.5	

boundary when upwind and also impacted by more emissions. In an attempt to account for these contributions of urban emissions at the upwind site, the regional background (PM_b) was determined by subtracting the predicted concentration (PM_p) from the observed concentration at the upwind site (PM_{up}) for each period. Table 7 also reveals that the resultant mean regional background derived with this method varied from 21.3 $\mu g/m^3$ at the CAM site to 37.2 $\mu g/m^3$ at the CLK site. The overall regional background of 32.4 $\mu g/m^3$ from all periods compares closely with 34 $\mu g/m^3$ determined by Batterman et al. (1986) from the lowest concentration for each period without consideration of the wind flow. The data base was sufficient in number to show that the regional particulate background is directionally dependent. This finding suggests that monitoring sites, strategically-located around an urban area, may be needed to accurately resolve the background particulate component for various flow regimes.

TABLE 7. OBSERVED AND MODEL PREDICTED PM_{10} AT UPWIND SITES

SITE UPWIND	N	PM_{up} ($\mu g/m^3$)	PM_p ($\mu g/m^3$)	Background (PM_b) ($\mu g/m^3$)	WIND DIR. (Deg.)	AND SPEED (m/s)
WTP	22	41.5±12.6	8.5±3.2	32.9	286±62	3.3
ARP	8	33.8±6.5	4.4±1.7	29.4	348±41	3.3
CAM	7	31.5±10.7	10.2±3.1	21.3	126±53	3.5
CLK	19	39.7±16.2	2.5±3.0	37.2	218±28	3.4
				32.4		

N - number of cases

MODEL EVALUATION STATISTICAL RESULTS

The statistical measures of difference and correlation between observed and modeled concentrations paired in time and location described by Fox (1981) were computed to evaluate model performance. The definitions for these measures and other statistical parameters are given in Appendix B. Two separate sets of statistical results were determined in this model evaluation. For Set 1, observations (O_i) were compared to the corresponding sum of model predictions and background (i.e. $P_i + PM_b$). For Set 2, results were obtained for model predictions (P_i) and corresponding resultant observed values derived by subtracting the background for each period from the measured concentration (i.e. $O_i - PM_b$).

The evaluation statistics in Table 8 contain the results from all sites for all periods (total), and separately for day and night cases. In this analysis where PM_b was included with predictions, paired values from the upwind site were omitted in the sample data set. Although this criterion reduced the sample size (N), the statistical measures would be artifically improved if upwind values were included due to the method of determining PM_b. Table 8 shows that PEM-2 slightly underestimated PM_{10} concentrations with an overall positive bias (d) of 5.3 $\mu g/m^3$. A value of 0.96 ± 0.3 for the ratio of P/O is favorable. However, measures of correlation from linear regression analysis depart from desired values. A relatively large intercept (A) of 23.7, a slope (b) of only 0.41, and a correlation coefficient (R) of 0.56 were determined from all available paired concentrations. Figure 5 shows that the few cases of high observed concentrations being greatly underpredicted had a definitive influence on the linear correlation measures and also effected the difference measures, such as bias. Nevertheless, a large majority of concentration pairs in Figure 5 are within a factor of 2 of each other. Several of the statistical results in Table 8 indicate that PEM-2 performed slightly better for the daytime periods as revealed by the lower bias, smaller mean squared error (MSE_d), and higher R. Interestingly, the correlation coefficients for PM_{10} are in between the higher values for FP and low values for CP in Ku and Rao (1986). However, it must be remembered that PM_b is a large factor in this set of concentrations pairs and its strong influence is reflected in these evaluation results.

The statistical results in Table 9 are presented to show how PEM-2 performed at each site for all periods. As in the previous analysis, concentration pairs at the upwind site were also excluded in these calculations. A notable outcome

TABLE 8. PEM-2 EVALUATION STATISTICS FOR PM_{10} (SET 1)

STATISTIC †	TOTAL	DAY	NIGHT
N	244	123	121
O	49.2±22.3	51.7±23.9	46.7±20.3
P*	43.9±16.4	47.3±18.0	40.4±13.9
Bias (d)	5.3	4.4	6.3
|d|	12.0	13.0	11.0
P*/O	0.96±0.3	1.0±0.3	0.92±0.3
S_d	19.0	18.8	19.2
A	23.7	22.8	26.9
b	0.41	0.47	0.29
R	0.56	0.63	0.42
MSE_u	185.1	193.0	156.7
MSE_s	201.2	176.1	247.0
MSE_d	386.3	369.1	403.8
MFE	0.7	0.5	0.9
IA	0.7	0.8	0.6

P* = P_i + Background
† - nomenclature and equations of statistical measures defined in Appendix B
Units are $\mu g/m^3$ for appropriate measures

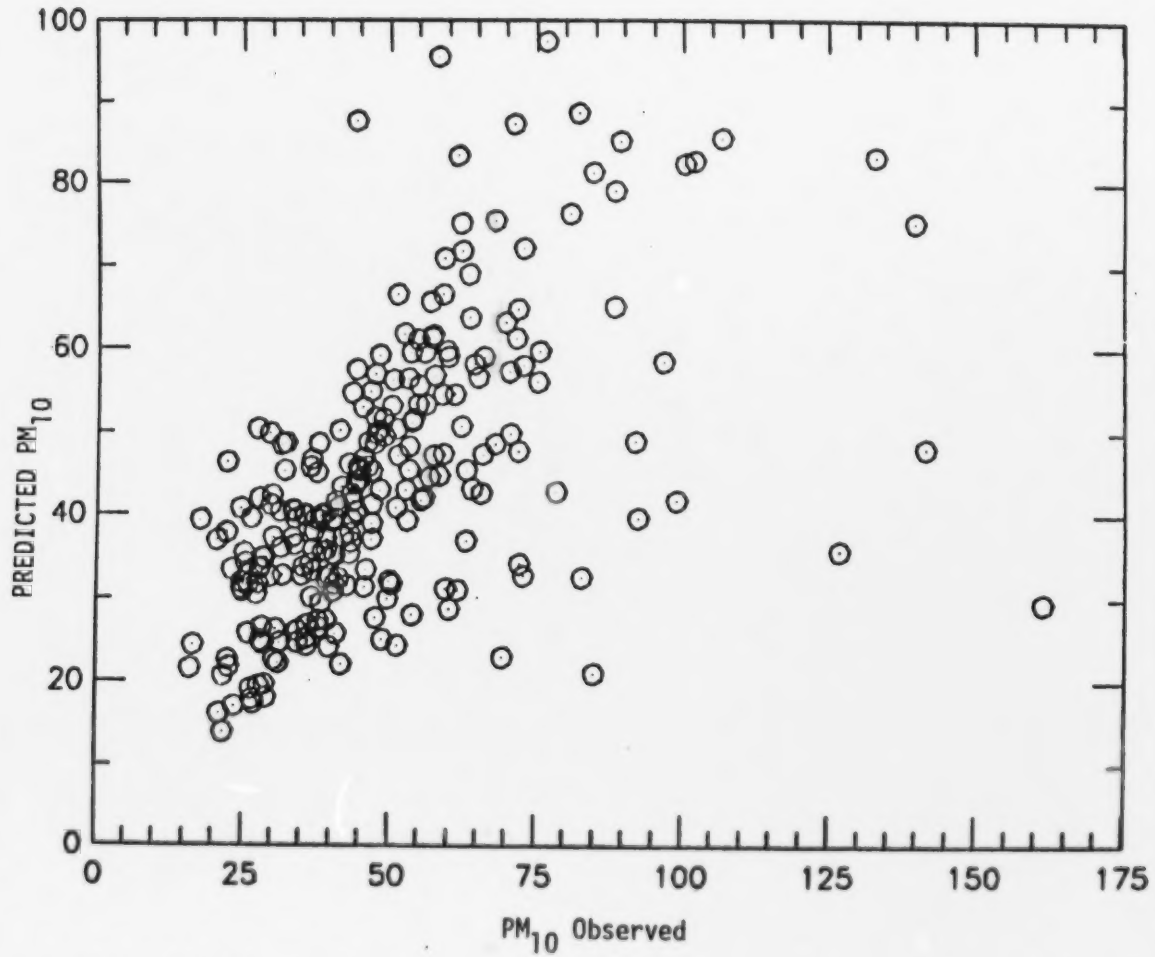

Figure 5. Observed versus model predicted (plus background) PM_{10} concentrations at all sites over all periods. The proposed 24-hour standard for PM_{10} is 150 ug/m^3.

is the poor model performance for site FRB, which is highlighted by the large positive bias and low correlation coefficient, although other statistical results also deviate strongly from those at the other sites. The fugitive dust sources are believed to have caused the high CP concentrations at site FRB. While mean CP concentrations were 50% or less of the mean FP values at the other sites for the study period, mean CP was slightly greater than FP at site FRB. It appears that the fugitive emissions may have been greatly underestimated in the inventory. Additionally, PEM-2 was not designed to treat subgrid scale sources of varying areal extent that differ from the larger uniform area grid size.

It is evident the high PM_{10} observations in Figure 5 occurred at site FRB. When all concentration pairs from site FRB were removed from the data set, several statistical measures improved dramatically. For example, model bias was reduced from 5.3 $\mu g/m^3$ to 0.7 $\mu g/m^3$, and R increased from 0.56 to 0.74.

Nevertheless, the dominant role of the background concentrations on this set of evaluation statistics has emerged. The percentages in the bottom line in Table 9 indicate that the magnitudes of the derived PM_b were about 70% or more of the measured PM_{10} concentrations, except at site FRB. Thus, the magnitude and variations in PM_{10} are primarily composed of a large regional background component at 5 of 6 PAFS sites with a smaller contribution due to urban sources.

Due to the large influence of PM_b on the previous evaluation statistics, the Set 2 of statistical results were obtained with concentration pairs composed of model predictions and resultant observed values minus the regional backgrounds. Several of the statistical measures in Table 10 reveal poor model performance as results differ largely from their values in Table 8. Although bias and absolute error d are nearly equivalent in both sets of results, their magnitudes represent a much greater fraction of the observed and predicted means in Table 10. Furthermore, correlation measures in Table 10 reveal a problem often encountered when evaluating a data set composed of relatively small values. Differences between small numbers are inherently magnified. The relatively large absolute error, near zero slope, and small R in Table 10 also indicate considerable scatter and little correlation between these paired concentrations. In fact, the standard deviations are comparable to the mean resultant observed values. These results also demonstrate the powerful role of the regional particulate background in this evaluation process. Consequently, model accuracy is difficult to discern as some statistical results differ based on how the background value is applied.

TABLE 9. STATISTICAL RESULTS FOR EACH PAFS SITE FOR PM_{10} (SET 1)

STATISTIC	SITE					
	BRD	FRB	WTP	ARP	CAM	CLK
N	36	50	31	44	48	35
O	45.7±16.0	67.4±31.0	46.6±18.6	47.3±15.8	45.4±17.4	36.8±13.5
P*	50.1±15.5	44.2±16.4	43.0±18.2	40.1±14.9	48.9±15.8	35.7±11.5
Bias (d)	-4.5	23.2	3.6	7.2	-3.5	1.0
d	7.9	24.7	9.2	9.8	9.1	7.5
P*/O	1.1±0.2	0.7±0.3	0.9±0.2	0.9±0.2	1.1±0.3	1.0±0.3
S_d	9.2	28.7	11.6	11.0	11.7	11.5
A	13.4	29.8	6.4	6.8	17.6	9.9
b	0.80	0.21	0.78	0.70	0.69	0.70
R	0.83	0.40	0.80	0.74	0.76	0.66
MSE_u	73.3	222.0	114.5	97.3	104.6	112.7
MSE_s	28.5	1121.1	28.6	72.8	40.8	16.8
MSE_d	101.8	1343.1	143.1	170.2	145.4	129.5
MFE	-0.7	2.9	0.6	1.1	-0.6	0.2
IA	0.9	0.6	0.9	0.8	0.8	0.8
PM_b/O	72%	48%	70%	69%	76%	85%

P* = P_i + background PM_b

TABLE 10. PEM-2 EVALUATION STATISTICS FOR PM_{10} (SET 2)

PARAMETER	TOTAL	DAY	NIGHT
N	240	120	120
O*	16.8±18.5	18.6±18.1	15.0±18.7
P	10.9±6.7	13.2±7.3	8.5±5.1
d	5.9	5.4	6.4
d	11.8	12.5	11.0
P/O*	1.4±7.4	1.6±8.9	1.3±5.6
S_d	18.5	17.9	19.1
A	9.8	11.5	8.3
b	0.06	0.09	0.01
R	0.18	0.23	0.06
MSE_u	43.3	50.0	25.6
MSE_s	332.7	297.1	379.4
MSE_d	376.0	347.1	404.9
MFE	0.5	-0.01	1.0
IA	0.4	0.4	0.3

where $O^* = O - PM_b$

An interesting feature evident in these sets of results is the reversal in magnitude of the unsystematic (MSE_u) and systematic (MSE_s) mean square errors. The large MSE_s values relative to MSE_u in Table 10 suggest model modifications are in order if improvement in model performance is desired. On the other hand, the large MSE_u in Table 8 reveals that errors are also unsystematic, which suggests modeled results may be the best that can be expected.

The statistical results for each site over all periods in Table 11 substantiate the poor model performance found earlier at site FRB. In particular, correlation coefficients are considerably lower, and even negative for site CLK, compared with those in Table 9. Distinctive features that appeared in both sets of results are overpredictions at sites BRD and CAM, and relatively large underpredictions at sites ARP and CLK, the most distant monitors from the city. These particular results are examined further in the next section where PEM-2 results are compared to RAM model predictions.

COMPARATIVE RESULTS FOR THE PEM-2 AND RAM MODELS

Both PEM-2 and RAM are Gaussian plume models with many of the same technical features and options. However, there are a few important differences between these models, which may yield variations in estimated concentrations. A relevant factor is that PEM-2 accounts for dry deposition and gravitational settling, while these processes cannot be considered by the RAM model. Another difference between these models is in the treatment of area emissions and their source heights. PEM-2 computes contributions from no more than eight upwind area cells to the concentration at a given receptor, while RAM can consider the impact at a particular receptor from all upwind area sources. Additionally, a single area source height can be specified in the PEM-2 runs. In contrast, RAM allows for input of different area source heights. Both models deal with area sources emissions according to the widely used narrow plume hypothesis.

The details of the RAM evaluation effort and results are documented in Anderson et al. (1986). Both models were executed with the same emissions data base, and hourly meteorological parameters, although there may be small differences in Z_i since Anderson et al. (1986) obtained observed values from a nearby rawinsonde site instead of using the airsonde data. Options for the RAM runs were set based on regulatory recommendations (EPA,1986).

TABLE 11. STATISTICAL RESULTS FOR EACH PAFS SITE FOR PM_{10} (SET 2)

STATISTIC	SITE BRD	FRB	WTP	ARP	CAM	CLK
N	36	50	30	44	47	33
O*	12.9±9.6	35.0±28.6	14.4±12.7	14.5±11.1	11.0±9.7	6.9±7.4
P	17.2±6.2	11.8±5.8	9.9±4.9	7.3±4.2	13.8±6.6	4.0±3.0
d	-4.3	23.2	4.5	7.2	-2.8	2.9
|d|	7.9	24.7	8.8	9.8	8.5	6.2
P/O*	3.4±9.6	0.6±0.8	0.5±3.4	-.1±4.1	3.8±13.3	0.0±1.8
S_d	9.2	28.7	10.8	11.0	10.6	8.2
A	14.1	11.2	6.8	6.2	12.4	4.2
b	0.24	0.02	0.22	0.08	0.13	-0.03
R	0.38	0.08	0.56	0.21	0.19	-0.07
MSE_u	31.4	32.2	16.2	16.8	41.0	8.6
MSE_s	70.5	1310.9	115.7	153.3	77.7	64.2
MSE_d	101.8	1343.1	131.9	170.1	118.7	72.8
MFE	-1.4	4.0	0.8	1.5	-1.3	-1.8
IA	0.6	0.4	0.6	0.5	0.4	0.3

where $O^* = O_i - PM_b$

A single area source height of 10 m was input in the PEM-2 model runs. In contrast, one of three possible source heights was specified for area sources in RAM; namely, 13.7 m, 9.1 m, or 4.6 m, were assigned to area sources based on emission rate (Anderson et al., 1986). The grid size for both models was 2.5 km. This means the contributions from area sources beyond 20 km from a site were not considered by PEM-2 in the concentration calculations for a given site. All area sources upwind of a site were included in RAM.

The statistical results from evaluations of both models are presented in Table 12. The RAM results are taken from Anderson et al. (1986). Their background values were added to the PEM-2 model results in this phase of the analysis to make the direct comparison with RAM possible. The sample sizes differ slightly between the model results because a 31-day period starting on 14 July was considered in the RAM evaluation. The common feature found from both sets of statistics in Table 12 is that PEM-2 predictions were consistently lower than RAM's results in the mean and peak concentrations. In the set where modeled predictions are considered alone, the PEM-2 mean value of 10.1 $\mu g/m^3$ is 3.1 $\mu g/m^3$ less, or about 75% of RAM's mean of 13.2 $\mu g/m^3$.

The model differences described earlier are believed responsible for the different predictions. Modeled concentrations by PEM-2 are reduced due to loss by deposition processes. RAM's consideration of more upwind areas sources and lower source heights for some area sources, particularly those grid cells outside the city, compared a uniform 10 m height for PEM-2 also contributed to higher concentrations since PEM-2 computations are limited to eight upwind area grids.

The relative similarity in results in Table 12 for both models make it difficult to state which model is superior or is more acccurate. While the correlation measures for PEM-2 are slightly better than the RAM results, the large positive biases reveal both models greatly underpredicted observed values. This indicates that attention should be focused on the background values derived by Anderson et al. (1986) because of the large contribution of PM_b to the total measured concentration described herein and by Batterman et al. (1986) with this PAFS data base. A mean PM_b of 20.5 $\mu g/m^3$ in Anderson et al. (1986) compares with 32.4 $\mu g/m^3$ presented in Table 7. The difference between these values is large enough to account for the significant model bias found in Table 12.

Anderson et al. (1986) derived the regional particulate component from the PAFS data after analyses of the lowest concentrations obtained every sixth day

TABLE 12. PEM-2 AND RAM MODEL RESULTS FOR PM_{10}

PARAMETER	PEM-2 (1)	RAM† (1)	PEM-2 (2)	RAM† (2)
N	305	318	305	318
O	47.4	47.5	26.9	26.9
P	30.6	33.8	10.1	13.2
d	16.8	13.7	16.8	13.7
A	17.6	21.6	8.2	11.7
b	0.27	0.26	0.07	0.06
R	0.56	0.52	0.19	0.13
MAX O	161.2	161.2	144.5	144.5
MAX P	58.3	71.3	35.4	49.1
2nd High				
O	101.8	101.8	76.1	76.1
P	57.9	63.1	35.4	43.0

(1) O_i versus $P_i + PM_b$ from Anderson et al. (1986)
(2) P_i versus $O_i - PM_b$ from Anderson et al. (1986)

† Results from Anderson et al. (1986)

for 1982 at one of 12 designated IP sites in a network surrounding Philadelphia. Measurements from this network were not utilized in the PEM-2 evaluations. However, different methods produced the large differences in PM_b, not the availability of additional measurement sites.

Separate statistical results are given in Table 13 to show model differences for each PAFS site. Both models performed poorly for site FRB. There were also large positive biases for both models at individual sites. PEM-2 results were lower than RAM predictions at each site. On the other hand, correlation coefficients and linear regression measures were slightly better for PEM-2 at most sites.

An interesting feature to be explored is the difference in model predictions for the various sites. Part 2 of Table 13 shows the model results differed by 5.2 $\mu g/m^3$ at site BRD to 2.6 $\mu g/m^3$ at site CLK. However, a more revealing result when comparing these model predictions is the ratio of this difference to the RAM prediction (i.e. $P_{RAM} - P_{PEM} / P_{RAM}$) at each site. Interestingly, the percentage of this ratio was about 20% for BRD site and at the 3 sites closest to it, but results jumped to 35% and 40% at sites ARP and CLK, respectively. These latter two sites are most distant from site BRD. It appears that differences between the models were accentuated when approaching the boundary of the model domain, which in this case is farthest from the city and important emissions. Further investigation of the models is required to determine the relative importance of the different factors in producing these differences. Nevertheless, it is clear that PEM-2 predicts lower PM_{10} concentrations than RAM, and the differences increased away from the city and also farther from the major emission sources.

Of particular relevance in regulatory applications is how a model simulates the highest concentrations since these are the values which may exceed a pollutant standard and provide the basis for the design concentration upon which a control strategy is implemented. Table 14 contains the high-5 modeled concentrations for both PEM-2 and RAM. The results are for predicted concentrations plus backgrounds from Anderson et al. and predictions without background. Results for these peak concentrations are similar to those obtained from the mean concentration results. PEM-2 predictions were almost always lower than RAM's results. The values of the ratio PEM-2/RAM were lowest at the 2 outermost sites, ARP and CLK. Both models significantly underpredicted the peak observed concentrations even when the regional background values of Anderson et al. (1986) were used. The PM_b values derived herein were generally much larger than those determined by Anderson et al., and their use would have eliminated the large positive bias.

TABLE 13. COMPARISION OF PEM-2 AND RAM FOR PM_{10} AT THE PAFS SITES

SET (1) P + PM_b from Anderson et al. (1986)

	SITE											
	BRD		FRB		WTP		ARP		CAM		CLK	
PARAMETER	PEM-2	RAM	PEM-2	RAM	PEM-2	RAM	PEM-2	RAM	PEM-2	RAM	PEM-2	RAM
N	36	37	51	53	55	57	53	55	56	59	54	57
O	45.7	45.7	66.8	66.8	44.9	45.4	45.8	46.3	44.0	43.7	37.8	37.9
P	37.3	42.4	31.9	34.8	30.2	32.5	27.4	31.2	34.4	37.8	24.4	27.1
d	8.4	3.3	34.9	32.0	14.7	12.9	18.5	15.1	9.5	5.9	13.4	10.8
A	16.3	21.4	24.7	28.8	8.5	14.8	7.3	8.6	16.0	19.6	7.6	11.7
b	.46	.46	.11	.09	.48	.39	.44	.49	.42	.42	.45	.40
R	.75	.68	.33	.30	.84	.73	.74	.76	.68	.68	.83	.72
SET (2) O - PM_b from Anderson et al. (1986)												
O	25.6	25.7	46.6	46.3	24.1	24.5	25.3	25.6	23.2	22.9	17.2	17.4
P	17.2	22.4	11.8	14.4	9.4	11.6	6.9	10.6	13.7	17.0	3.9	6.5
P Diff	5.2		2.6		2.2		3.7		3.3		2.6	
A	14.4	19.2	11.4	14.4	4.9	10.7	4.8	5.9	13.4	15.9	5.6	8.3
b	0.11	0.12	0.01	-0.00	0.19	0.04	0.08	0.18	0.01	0.05	-.10	-.10
R	0.18	0.16	0.04	-0.00	0.49	0.10	0.22	0.37	0.02	0.08	-.21	-.14

P Diff = RAM - PEM-2 prediction

TABLE 14. COMPARISON OF THE HIGH-FIVE PM_{10} CONCENTRATIONS FOR PEM-2 AND RAM

MAXIMUM	BRD (1)	BRD (2)	FRB (1)	FRB (2)	WTP (1)	WTP (2)	ARP (1)	ARP (2)	CAM (1)	CAM (2)	CLK (1)	CLK (2)	6-SITE AVE. (2)
PEM-2	55.2	30.9	58.3	28.4	57.9	24.7	51.8	20.8	57.0	35.4	40.6	15.0	25.9
RAM	71.3	49.1	63.1	40.9	57.8	27.7	62.2	29.0	63.1	43.0	45.7	23.5	35.5
2ND HIGH													
PEM-2	53.1	29.8	51.0	27.8	51.8	19.4	48.7	16.1	54.1	28.0	39.4	14.7	22.6
RAM	64.6	37.1	60.9	26.1	51.0	27.0	56.4	26.8	61.9	33.6	44.2	21.0	28.6
3RD HIGH													
PEM-2	50.6	27.3	49.4	24.2	48.5	17.0	46.2	15.7	52.6	25.9	37.8	13.7	20.6
RAM	63.4	33.4	59.9	25.3	49.9	22.4	56.1	23.4	55.8	32.1	41.4	20.4	26.2
4TH HIGH													
PEM-2	49.5	26.3	48.2	21.8	45.1	16.0	45.7	14.1	52.2	25.3	37.3	11.5	19.2
RAM	61.7	32.8	56.1	24.5	49.4	22.2	51.2	21.1	54.8	29.6	39.9	20.6	25.1
5TH HIGH													
PEM-2	48.9	25.0	46.8	19.8	44.7	15.5	41.2	13.3	50.4	24.9	36.8	10.3	18.1
RAM	60.3	31.6	50.9	24.3	48.1	21.9	47.5	20.8	53.5	27.5	39.4	18.3	24.1
HIGH-5 AVE.													
PEM-2	51.5	27.9	50.7	24.4	49.6	18.5	46.7	16.0	53.3	27.9	38.4	13.0	21.3
RAM	64.3	36.8	58.2	28.2	51.2	24.2	54.7	24.2	57.8	33.2	42.1	20.8	27.9
RATIO													
PEM-2/RAM	0.80	0.76	0.87	0.86	0.97	0.76	0.85	0.66	0.92	0.84	0.91	0.62	0.76
HIGH-5 Obs. AVE.	73.7	44.1	140.3	114.9	80.5	51.3	79.4	50.8	80.0	47.5	70.4	36.9	

(1) P + background
(2) P without background added

SECTION 4

SUMMARY AND CONCLUSIONS

An evaluation of the PEM-2 urban dispersion-deposition model has been performed with measurements from the 1982 Philadelphia Aerosol Field Study data base. Observed and model predicted 12-hour PM_{10} concentration pairs were statistically evaluated to determine model performance over a 29-day study period. Analysis of the observed concentrations from 6 monitoring sites indicated the regional particulate background was a large contributor to urban PM_{10} concentrations in Philadelphia, as the mean PM_{10} concentrations from concurrent measurements at these sites differed by only 10 $\mu g/m^3$. Consequently, the method to derive regional background values consisted of consideration of the wind flow and contribution from urban emissions at the upwind site. Regional background component was found to be about 70% or more of the measured PM_{10} concentration at 5 of 6 sites. The remaining urban site was strongly impacted by local fugitive emissions.

Statistical results were computed from two sets of concentration pairs; modeled plus background versus observed, and modeled only versus observed minus background. Better performance was obtained when background values were added to model predictions; however, these results were greatly influenced by the large regional background values. For the other set, large errors and little correlation was found from the modeled and resultant observed values minus background since magnitudes were relatively small. Therefore, model performance and accuracy was difficult to judge because of the dominant role of background for this data set.

A comparison of PEM-2 and RAM model results was conducted by applying the regional background values derived for the RAM evaluation. Results revealed that PEM-2 predictions were lower than RAM concentrations both for mean and peak values. The factors responsible for lower PEM-2 concentrations include; loss of mass by dry deposition and gravitational settling processes simulated by PEM-2 which were not treated in RAM, and different methods to handle area source emissions and area heights. PEM-2 considers the contributions from up

to 8 upwind area sources, while all upwind area sources were included in computations by RAM. The relative importance of these factors was not assessed, but deserves further investigation.

Large positive biases in the comparision of PEM-2 and RAM results may be explained by regional backgrounds too low due to the method used by Anderson et al. (1986). The PM_{10} background concentrations derived for and used in the PEM-2 evaluation were considerably larger than those computed by Anderson et al. (1986). The latter were used in the RAM model evaluation and were also added to the PEM-2 results for the purpose of the model comparison. Otherwise, the strong similarity in the statistical results revealed little evidence to distinguish between the performances of these models. Model accuracy was also difficult to assess from the evaluation statistics due to the dominant role of the regional background component. Future evaluations are necessary to adequately assess the impact of deposition processes for urban particulate applications.

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APPENDIX A

EVALUATION OF MODELED MIXING HEIGHTS WITH PAFS OBSERVATIONS

Mixing heights derived from two different methods were statistically evaluated against observed values at 1000 LDT. It is acknowledged that the sample size of 29 is relatively small and the evaluation is limited in extent to a particular hour. However, this effort was undertaken with the intentions of obtaining some valuable evidence to distinguish between the two methods and to determine how accurately Z_i can be simulated for this rapidly changing time period.

Two sets of urban Z_i's were computed; from the RAMMET pre-processor program and by an empirical equation developed by Godowitch et al. (1985). The hourly mixing heights for the PEM-2 evaluation were provided by RAMMET. It's technique is to derive Z_i by linear interpolation between local sunrise and 1400 LST with observed morning minimum and afternoon maximum values. The other method is an empirical mixing heights growth equation derived from a second order least square regression fit to a large data set from St. Louis, Missouri. The empirical urban Z_i growth equation, in a slightly modified form from Godowitch et al. (1985), is given by

$$Z_i(t) = Z_i(o) - 7.0t + 24.3\ t^2 \qquad \text{(A-1)}$$

where $Z_i(o)$ is the urban mixing height at sunrise for a particular day and t is in hours after sunrise. Equation (A-1) is only applicable between sunrise and the time when the nocturnal inversion is destroyed, which usually occurs around mid-morning. According to Equation A-1, urban mixing height growth is distinctly nonlinear during this time period. The destruction of the nocturnal inversion layer marks the end of the morning transition period. It is followed by a relatively short period of more rapid, even explosive, growth that often occurs through a thicker overlying layer of much weaker stability until the mixing height of the previous afternoon is reached. It is likely that the observations at 1000 LDT were obtained under both stages, as the mean time of complete inversion destruction in St. Louis was around this hour.

The results of statistical analysis for both methods are shown in Table A-1. A large negative bias was found for the RAMMET model. In fact, it's values overpredicted observations in 24 of 29 cases. The results from Equation (A-1) showed more balance with a small negative bias. There were 17 overpredictions

and 12 underpredicitons with this model. In addition, the results for the average absolute error and mean P/O were more favorable with Equation (A-1). On the otherhand, the linear regression measures of slope and intercept suggested a slightly better correlation between RAMMET and observed pairs. However, the total mean square error (MSE_d) in the RAMMET results is dominated by a large systematic component (MSE_s), which suggests model revision is necessary if performance is to be improved.

Thus, even though a mixed picture appears when considering all the statistical measures, the results for Equation (A-1) are better than RAMMET's for most of the statistical parameters. The large standard deviations for the observations demonstrates the amount of variability in Z_i during this time of rapid change. Nevertheless, a tentative conclusion from this limited evaluation data set is that RAMMET often overpredicts urban mixing heights at this time period. Additional evaluations with larger data sets are needed to confirm these results.

TABLE A-1. STATISTICAL RESULTS OF MIXING HEIGHT MODEL EVALUATIONS

PARAMETER	METHOD	
	RAMMET	EQUATION (A-1)
N	29	29
O	641.4 ± 282.8	641.4 ± 282.8
P	917.4 ± 182.3	675.9 ± 215.5
d	-276.0	-34.5
|d|	313.8	240.6
P/O	1.7 ± 0.7	1.3 ± 0.6
A	711.6	538.0
b	0.32	0.22
R	0.50	0.28
MSE_u/MSE_d	17.8%	45.8%
MSE_s/MSE_d	82.2%	54.2%

APPENDIX B

DEFINITIONS OF STATISTICAL MEASURES

The nomenclature and equations for the various statistical measures used to determine model performance are given. The measures of difference and correlation are computed from N samples of individual observations (O_i) and model predictions (P_i). Means and standard deviations for observed and predicted values were computed from standard formulas. Measures of difference are based on residuals between observed and predicted concentrations where;

Bias $$d_i = o_i - P_i \tag{B-1}$$

$$\overline{d} = \frac{1}{N} \Sigma d_i \tag{B-2}$$

average absolute gross error $$|\overline{d}| = \frac{1}{N} \Sigma |d_i| \tag{B-3}$$

standard deviation of bias $$S_d = \left[\frac{1}{N-1} \Sigma (d_i - d)^2\right]^{1/2} \tag{B-4}$$

Measures of correlation between O_i and P_i from linear regression analysis include the intercept (A), slope of a line (b) and correlation coefficient (R). These measures are computed by;

$$b = \frac{\Sigma (O_i' X P'_i)}{\Sigma O_i'^2} \tag{B-5}$$

where $O'_i = O_i - \overline{O}$ and $P'_i = P^i - \overline{P}$, the differences between observed and predicted values and their means.

$$a = \overline{P} - b\overline{O} \tag{B-6}$$

$$R = \frac{\Sigma(O_i' X P_i')}{\left[\Sigma O_i'^2 \Sigma P_i'^2\right]^{1/2}} \tag{B-7}$$

The estimate of a prediction PE_i is given by

$$PE_i = a + b\ O_i \tag{B-8}$$

The unsystematic (MSE_u) and systematic (MSE_s) components of the mean square error are given by

$$MSE_u = \frac{1}{N} \Sigma(P_i - PE_i)^2 \quad \text{and} \tag{B-9}$$

$$MSE_s = \frac{1}{N} \Sigma(PE_i - O_i)^2, \text{ respectively.} \tag{B-10}$$

The mean square error of the differences (MSE_d) is computed from;

$$MSE_d = \frac{1}{N} \Sigma d_i^2 \tag{B-11}$$

Mean fraction error (MFE) is an indicator of the model's overall bias to underpredict or overpredict.

$$MFE = \frac{1}{N} \Sigma \frac{d_i}{((O_i + P_i)/2)^{1/2}} \tag{B-12}$$

The index of agreement (IA) is given by;

$$IA = \frac{1 - \Sigma\ d_i^2}{\Sigma\ [|P_i - \overline{o}| + |o_i|]^2} \tag{B-13}$$

APPENDIX C

OBSERVED AND PEM-2 MODEL PM_{10} CONCENTRATIONS

A listing of corresponding 12-hour average observed (O) and predicted (P) concentrations at each site is given for the 29-day period from the PAFS program. The model evaluation period for the PEM-2 study was from 16 July through 13 August 1982. Missing values are designated by 999. The time (local daylight time, LDT) represents the starting hour of the averaging period.

DATE (M/D)	TIME (LDT)	BRD P	BRD O	FRB P	FRB O	WTP P	WTP O	ARP P	ARP O	CAM P	CAM O	CLK P	CLK O
7/16	06	28.6	999.0	17.4	999.0	19.4	999.0	8.9	999.0	14.2	57.3	1.2	34.1
7/16	18	27.6	999.0	18.6	999.0	16.4	72.6	11.6	999.0	21.6	61.3	2.5	999.0
7/17	06	26.5	999.0	27.8	57.2	24.7	96.5	20.8	60.8	28.0	52.3	1.5	35.2
7/17	18	16.2	52.8	13.2	38.7	6.5	45.9	8.1	40.7	15.6	29.8	1.5	28.3
7/18	06	20.1	999.0	18.0	75.4	15.5	57.1	15.7	70.2	19.6	71.4	1.1	65.5
7/18	18	8.4	999.0	6.4	999.0	4.4	71.7	4.7	88.3	11.4	62.0	1.2	61.5
7/19	06	23.5	51.2	19.2	999.0	12.6	55.6	16.1	65.7	22.6	56.8	1.6	56.7
7/19	18	13.3	51.0	7.9	999.0	6.3	43.3	5.0	55.7	9.7	45.5	2.4	40.5
7/20	06	23.3	46.7	21.8	56.0	8.8	40.3	14.0	44.6	23.1	43.3	4.0	38.4
7/20	18	21.6	31.4	12.8	33.9	10.4	39.1	6.5	33.2	14.0	24.4	4.8	26.0
7/21	06	16.5	27.8	10.3	39.1	9.5	28.2	3.6	29.0	14.0	17.7	8.0	23.1
7/21	18	13.0	999.0	5.8	40.9	5.8	25.8	2.9	69.3	7.6	47.6	2.7	22.4
7/22	06	14.7	999.0	12.4	82.9	8.0	28.2	4.2	35.9	15.6	36.8	10.3	27.2
7/22	18	13.5	999.0	7.2	60.1	6	28.2	3.5	48.8	9.6	59.4	2.9	51.4
7/23	06	26.3	62.0	24.2	67.8	15.6	999.0	7.3	50.5	25.3	47.7	14.7	39.0
7/23	18	27.3	47.4	14.1	43.1	16.0	37.2	9.5	40.3	14.7	999.0	2.8	999.0
7/24	06	16.7	999.0	12.6	34.6	7.8	28.9	5.8	45.6	15.4	999.0	9.6	999.0
7/24	18	9.0	999.0	5.0	39.7	5.4	34.4	2.9	41.8	5.3	28.5	1.5	20.7
7/25	06	16.7	999.0	16.4	51.1	15.4	35.5	12.4	63.1	16.8	46.9	9.6	34.1

DATE (M/D)	TIME (LDT)	BRD		FRB		WTP		ARP		CAM		CLK	
		P	O	P	O	P	O	P	O	P	O	P	O
7/25	18	7.1	53.7	5.7	70.4	3.2	59.1	3.3	65.7	8.9	50.2	1.1	45.2
7/26	06	12.8	67.6	12.7	139.5	8.0	70.5	9.5	72.6	13.7	80.4	1.2	63.5
7/26	18	13.2	61.9	7.1	63.3	6.3	68.0	4.8	58.8	9.1	59.1	1.5	69.6
7/27	06	16.7	54.6	11.0	71.8	9.0	46.3	5.0	43.7	14.3	50.9	7.0	44.2
7/27	18	16.2	999.0	8.2	55.8	8.2	53.4	5.1	52.9	8.3	59.6	1.8	53.1
7/28	06	11.0	999.0	7.3	132.7	7.4	61.3	3.8	999.0	6.8	101.8	.9	76.7
7/28	18	19.1	999.0	11.3	161.2	13.0	31.1	8.0	34.2	11.9	36.6	1.5	28.8
7/29	06	15.4	27.8	11.4	38.2	7.5	25.5	3.7	22.7	19.7	22.2	6.4	16.5
7/29	18	14.2	32.3	7.3	99.0	6.8	41.2	3.5	37.2	10.8	31.9	2.5	20.6
7/30	06	30.9	46.8	28.4	78.4	17.0	45.7	12.5	35.9	35.4	29.5	11.5	25.8
7/30	18	17.3	40.2	11.6	999.0	11.3	36.8	9.0	24.9	10.2	32.1	.7	30.4
7/31	06	19.0	999.0	10.5	64.9	10.8	47.3	5.5	53.9	10.1	50.4	1.1	47.1
7/31	18	20.2	54.9	11.7	51.4	10.1	62.9	6.5	55.3	14.0	48.9	4.6	39.9
8/01	06	10.5	44.8	10.7	53.3	6.8	41.5	5.7	33.3	11.8	36.7	4.5	38.1
8/01	18	5.8	41.3	3.9	46.8	3.1	38.3	1.6	43.4	5.2	44.4	2.0	33.4
8/02	06	22.9	48.1	19.8	75.2	10.4	46.6	9.8	42.9	24.9	54.5	8.0	44.9
8/02	18	18.0	999.0	9.1	141.5	8.4	47.2	6.2	37.5	12.8	47.3	3.6	43.4
8/03	06	16.0	999.0	10.9	126.7	7.8	39.6	5.0	29.8	14.7	37.3	7.5	39.3
8/03	18	13.1	999.0	5.9	64.0	6.2	41.8	3.0	40.1	7.5	58.4	2.5	43.5
8/04	06	25.0	76.6	16.1	82.0	14.8	70.9	5.3	77.7	23.1	58.1	15.0	44.2

DATE (M/D)	TIME (LDT)	BRD P	BRD O	FRB P	FRB O	WTP P	WTP O	ARP P	ARP O	CAM P	CAM O	CLK P	CLK O
8/04	18	19.3	58.7	11.0	64.1	10.8	72.6	7.3	58.7	11.9	59.7	2.6	49.6
8/05	06	16.7	100.2	19.8	106.5	19.4	89.2	13.3	88.1	15.6	84.5	.9	66.5
8/05	18	20.0	57.0	15.5	57.4	10.2	51.5	10.1	48.8	16.2	44.2	1.6	48.3
8/06	06	13.0	47.0	10.2	72.0	8.1	49.9	7.6	42.6	12.7	36.6	3.4	39.3
8/06	18	19.1	25.8	8.6	31.1	12.7	30.6	4.4	28.9	10.0	23.7	2.5	20.9
8/07	06	21.9	999.0	11.2	35.9	12.3	38.1	3.7	26.6	9.2	24.3	5.4	27.8
8/07	18	9.0	31.2	5.4	85.0	5.2	21.6	3.5	26.3	6.0	16.0	.8	16.4
8/08	06	14.2	26.3	15.7	29.7	10.7	31.6	12.0	30.1	15.1	33.5	1.2	26.5
8/08	18	5.2	999.0	4.8	999.0	4.1	36.3	2.8	31.8	4.2	34.2	.3	999.0
8/09	06	8.5	999.0	5.8	41.4	5.1	40.7	3.4	49.7	6.2	34.9	.9	27.5
8/09	18	14.8	999.0	10.7	41.9	8.7	999.0	8.7	40.4	13.2	38.3	.9	27.5
8/10	06	11.8	46.2	12.1	91.9	7.1	44.0	8.9	36.5	13.3	48.0	.9	43.1
8/10	18	12.5	45.2	7.9	53.3	6.1	46.4	5.5	44.6	9.7	41.4	1.2	40.8
8/11	06	13.7	29.7	9.2	53.8	6.4	25.3	4.0	999.0	13.0	24.8	6.1	28.0
8/11	18	17.3	28.3	7.9	23.6	8.3	26.8	4.1	999.0	9.8	18.9	4.7	21.7
8/12	06	8.4	33.8	4.8	72.9	3.7	27.6	1.7	29.6	5.7	28.0	3.3	24.7
8/12	18	16.5	37.9	7.3	53.0	7.9	38.6	3.5	35.6	7.9	35.4	2.8	28.8
8/13	06	29.8	27.3	19.2	92.5	14.9	25.1	6.5	26.9	25.9	22.2	13.7	25.5
8/13	18	17.9	31.3	8.5	61.6	8.7	31.2	4.8	37.9	11.2	35.2	3.2	25.8